The metabolism of *Escherichia coli* as a multiparametric programming problem

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The widely studied metabolism of *Escherichia coli* consists of a complex myriad of intracellular reaction pathways. In genome-scale metabolic models, this intracellular reaction network is reconstructed from information in the cellular genome. Flux balance analysis (FBA) is used to determine the metabolic flux distribution over these intracellular reaction pathways according to a specific cellular objective. Incorporation of this mechanistic information in metabolic models increases model accuracy and genericness. These metabolic models can be integrated in single-cell models for the simulation of individual cellular behavior. However, the addition of model complexity increases the required simulation run time as well, especially for individual-/agent-based models (IbM/AbM) in which the cells in a microbial population are simulated as individual agents. In addition, the cellular objective is dependent on the environmental conditions to which the cell is exposed, turning the determination of the *E. coli* metabolism in a multiparametric programming problem. For this reason, a noncomplex linear metabolic model has been developed that (*i*) is calibrated by means of flux balance analyses with a genome-scale model, (*ii*) omits superfluous information about intracellular reaction fluxes, considering the cell as a black box taking up nutrients and secreting cell products, (*iii*) takes into account the influence of pH and weak acid cell products on the *E. coli* metabolism.